Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

The effect of substituted 1,2,4-triazole moiety on the emission, phosphorescent properties of the Blue emitting hetroleptic iridium (III) complexes and the OLED performance: a theoretical study

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Supplementary Table 1: Main optimized geometry structural parameters of 1-5 in ground state along with the experimental values

Bond-length(Å)									
	1		**2**	**3**		**4**		**5**	
	EXP	**THEO**	**THEO**	**EXP**	**THEO**	**EXP**	**THEO**	**EXP**	**THEO**
Ir-N1	-	2.047	2.048	2.057	2.048	2.046	2.047	2.023	2.049
Ir-N2	-	2.045	2.046	2.045	2.047	2.036	2.047	2.034	2.045
Ir-C3		2.009	2.008	2.013	2.007	2.006	2.008	2.016	2.007
Ir-C4		1.996	1.996	1.997	1.996	2.017	1.997	1.989	1.996
Ir-N5		2.117	2.116	2.168	2.204	2.128	2.119	2.172	2.206
Ir-N6		2.203	2.202	2.127	2.120	2.156	2.204	2.108	2.122
Bond-Angle(deg)									
N5-Ir-N6		76.0	76.0	76.4	76.2	76.7	76.9	76.7	76.9
C1-Ir-N1		80.5	80.5	80.0	80.3	80.4	80.7	80.5	80.3
C2-Ir-N2		80.5	80.5	80.0	80.5	80.3	80.5	80.2	80.1

Supplementary Table 2: Mulliken charges of important atoms in the 1-5 complexes

Atom	1	2	3	4	5
Ir	1.006496	1.010218	1.008157	1.008915	1.005629
C1	-0.217508	-0.240587	-0.241242	-0.241227	-0.218715
N1	-0.633124	-0.634501	-0.634157	-0.634416	-0.634918
C2	-0.241650	-0.218369	-0.218727	-0.218381	-0.218715
N2	-0.634848	-0.633261	-0.633422	-0.633509	-0.632391
N3	-0.434059	-0.427154	-0.424553	-0.425773	-0.428257
N4	-0.548783	-0.549736	-0.548003	-0.548661	-0.546212

Supplementary Table 3: The calculated HOMO-LUMO gap (Δ_{H-L}) and the lowest excitation energies (E_g) for 1-5.

Complex	Δ_{H-L} (eV) cal	E_g (eV) cal
1	3.67	3.75
2	3.57	3.64
3	3.85	3.86
4	3.90	3.91
5	4.00	3.98

Supplementary Table 4: Molecular orbital composition for 1-5 in the ground state

Complex	MO	Composition				Characteristics
1		**Ir**	**(F_2ppy)**	**(F_2ppy)**	**(pta)Me**	
	H-5	47.1	16.2	17.6	19	π(F_2ppy)+Ir(d)
	H-4	38.9	29.9	17	14.2	π(F_2ppy)+Ir(d)
	H-3	23.8	2.7	56	17.5	π(F_2ppy)+Ir(d)
	H-2	8.7	8.7	10.2	72.3	π(pta)Me
	H-1	27.4	58.1	7.1	7.4	π(F_2ppy)+Ir(d)
	H	43.8	11.6	16.3	28.2	π pta(Me)+Ir(d)
	L	4.2	12.7	78.8	4.3	π*(F_2ppy)
	L+1	5.7	74.6	12	7.7	π*(F_2ppy)
	L+2	6	9.5	2.9	81.6	π*(pta)Me
	L+3	2.5	36.8	43.9	16.8	π*(F_2ppy)
	L+4	2.6	22.2	50.5	24.7	π*(F_2ppy)
	L+5	1.7	39.9	2.6	55.8	π*(F_2ppy+ptaMe)
		Ir	**(F_2ppy)**	**(F_2ppy)**	**(pta)PhOMe**	
2	H-5	1.7	39.9	2.6	55.8	π (F_2ppy+PhoMe)
	H-4	4.5	1.8	6.1	87.7	π(PhoMe)
	H-3	16.2	25	43	15.8	π(F_2ppy)
	H-2	26.6	15.6	23.3	34.5	π(PhoMe)+Ir(d)
	H-1	24.5	54.4	9.4	11.7	π(F_2ppy)+Ir(d)
	H	44.6	32.3	19.5	3.6	π(F_2ppy)+Ir(d)
	L	5.5	0.8	1.7	91.9	π*(PhOMe)
	L+1	4.4	5	82	8.6	π*(F_2ppy)
	L+2	5.2	22.2	9.6	63	π*(PhoMe)
	L+3	6	66.3	2.3	25.4	π*(PhoMe+ F_2ppy)
	L+4	2.5	18.7	46.6	32.1	π*(PhoMe+F_2ppy)
	L+5	2.7	37.3	45.4	14.6	π*(F_2ppy)
		Ir	**(F_2ppy)**	**(F_2ppy)**	**pta(4Fph)**	
3	H-5	1.6	41.3	4.8	52.2	π (4Fph)
	H-4	51.6	15.3	11.3	21.8	π(4Fph)+Ir(d)
	H-3	21.3	16.9	59.4	2.4	π(F_2ppy)
	H-2	1.4	2.3	0.3	96.1	π(4Fph)
	H-1	12	72.6	11	4.4	π(F_2ppy)
	H	39.9	30.2	17.6	12.3	π(F_2ppy)
	L	19.4	4.3	4.5	71.7	π*(4Fph)
	L+1	4.4	4.5	84.7	6.4	π*(F_2ppy)
	L+2	4.8	3.5	4.6	87.1	π*(4Fph)

	L+3	5.7	85.5	3.9	4.8	π*(F_2ppy)
	L+4	2.6	9.8	36.3	51.2	π*(4Fph)
	L+5	2.6	3	59.7	34.7	π*(F_2ppy+4Fph)
		Ir	**(F_2ppy)**	**(F_2ppy)**	**pta(3,5FPh)**	
4	H-5	2.3	84.1	2.4	11.2	π (F_2ppy)
	H-4	41.6	10	14.7	33.8	π(3,5FPh)+Ir(d)
	H-3	46.6	16.2	12.4	24.8	π(F_2ppy)+ Ir(d)
	H-2	20.5	15.2	56.3	7.9	π(F_2ppy)
	H-1	14	66.5	14.5	4.9	π(F_2ppy)
	H	43.9	31.5	20	4.7	π(F_2ppy)
	L	9.4	1.1	2.1	87.4	π *(3,5FPh)
	L+1	4.3	4	63.5	28.2	π*(F_2ppy)
	L+2	5.3	5	9.9	79.8	π*(3,5FPh)
	L+3	5.8	63	21.8	9.5	π*(F_2ppy)
	L+4	2.4	15.5	39.4	42.7	π*(F_2ppy)
	L+5	2.6	22.3	50.6	24.4	π*(F_2ppy)
		Ir	**(F_2ppy)**	**(F_2ppy)**	**pta(F_5Ph)**	
5	H-5	1.8	53.1	6.3	38.8	π (F_2ppy+ F_5Ph)
	H-4	46.3	12.9	17.2	23.7	π(F_2ppy)+Ir(d)
	H-3	20.9	17.4	58	3.7	π(F_2ppy)
	H-2	10.1	75.3	11	3.6	π(F_2ppy)
	H-1	0	0	0	100	π(F_5Ph)
	H	38.7	37.4	16.7	7.2	π(F_2ppy)
	L	13.3	3	3.1	80.7	π*(F_5Ph) +Ir(d)
	L+1	3.7	3	59.5	33.8	π*(F_2ppy)
	L+2	6.2	2.4	29.9	61.5	π*(F_5Ph)
	L+3	5.7	88.5	3.5	2.4	π*(F_2ppy)
	L+4	2.1	19.5	33	45.4	π*(F_5Ph)
	L+5	2.5	14.7	62	20.8	π*(F_2ppy)